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N-[(3-Ethylphenyl)carbamothioyl]-2,2-diphenylacetamide

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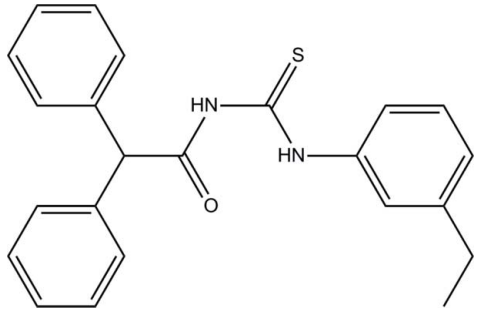
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.098; data-to-parameter ratio = 16.3.

In the title molecule, $C_{23}H_{22}N_2OS$, the diphenylacetyl and ethylbenzene groups adopt a *trans–cis* conformation, respectively, with respect to the S atom across the (S=)C—N bonds. This conformation is stabilized by an intramolecular N—H···O hydrogen bond and a weak C—H···S hydrogen bond. The ethyl-substituted benzene ring forms dihedral angles of 87.53 (15) and 73.94 (15)° with the phenyl rings. In the crystal, N—H···O hydrogen bonds link molecules into chains along [100]. A weak C—H···π interaction is also observed.

Related literature

For the biological activity of carbonylthiourea derivatives, see: Zhong *et al.* (2008); Saeed *et al.* (2010). For related structures, see: Yusof *et al.* (2012*a*,*b*). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986). For standard bond lenths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{23}H_{22}N_2OS$
M_r = 374.49
Orthorhombic, $Pna2_1$
a = 10.0608 (2) Å
b = 17.9092 (5) Å
c = 10.8495 (3) Å
V = 1954.87 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 100 K
0.26 × 0.23 × 0.09 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.955, T_{max} = 0.983
11560 measured reflections
4121 independent reflections
2885 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.098
S = 0.99
4121 reflections
253 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 1761 Friedel pairs
Flack parameter: 0.17 (9)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1*N2*···O1	0.90 (3)	1.82 (3)	2.630 (3)	148 (3)
C21—H21*A*···S1	0.95	2.61	3.255 (3)	126
N1—H1*N1*···O1^{i}	0.82 (3)	2.25 (3)	3.023 (3)	157 (3)
C7—H7*A*···*Cg*^{ii}	1.00	2.87	3.844 (3)	166

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z$; (ii) $-x-\frac{1}{2}, y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5616).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2009). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Saeed, S., Rashid, N., Jones, P. G., Ali, M. & Hussain, R. (2010). *Eur. J. Med. Chem.* **45**, 1323–1331.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

‡ Thomson Reuters ResearcherID: F-9119-2012.
§ Thomson Reuters ResearcherID: A-5599-2009.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Yusof, M. S. M., Arshad, S., Razak, I. A. & Rahman, A. A. (2012*b*). *Acta Cryst.* E**68**, o2670.
Yusof, M. S. M., Mutalib, S. F. A., Arshad, S. & Razak, I. A. (2012*a*). *Acta Cryst.* E**68**, o982.
Zhong, Z., Xing, R., Liu, S., Wang, L., Cai, S. & Li, P. (2008). *Carbohydr. Res.* **343**, 566–570.

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S1. Comment

Carbonylthiourea derivatives have been explored because they are reported to posses biological activities such as antibacterial, anti-fungal and antiviral (Zhong *et al.*, 2008; Saeed *et al.*, 2010). The crystal structure of the title compound is presented herein.

The molecular structure is shown in Fig. 1. The diphenylacetyl and ethylbenzene groups adopt a *trans-cis* configuration, respectively, with respect to the sulfur atom across the (S═)C–N bonds. Intramolecular N2—H1N2···O1 and C21—H21A···S1 hydrogen bonds result in two *S*(6) graph-set motifs (Bernstein *et al.*, 1995). The ethyl-substituted benzene ring (C16–C21) forms dihedral angles of 87.53 (15) and 73.94 (15)°, respectively with the C1–C6 and C8–C13 rings. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and comparable to related structures (Yusof *et al.*, 2012*a*,*b*).

In the crystal molecules are linked into one-dimensional chains along the [100] via intermolecular N1—H1N1···O16^{i} hydrogen bonds (Table 1). In addition, a weak C7—H7A···*Cg*^{ii} interaction is observed (*Cg* is the centroid of C8–C13).

S2. Experimental

An acetone (30 ml) solution of 3-ethylaniline (1.63 g, 13.5 mmol) was added to a round-bottom flask containing 2,2-diphenylacetyl chloride (3.10 g, 13.5 mmol) and ammonium thiocyanate (1.03 g, 13.5 mmol). The mixture was refluxed for 2.5h then filtered off and left to evaporate at room temperature. The colourless precipitate obtained was washed with water and cold ethanol. Colourless crystals suitable for X-ray analysis were obtained by recrystallization of the precipitate in DMSO.

S3. Refinement

N-bound H atom were located in difference maps and refined freely, [N–H = 0.82 (3) and 0.90 (3) Å]. The remaining H atoms were positioned geometrically [C–H = 0.95–1.00 Å] and refined using a riding model with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C). A rotating group model was applied to the methyl group. In the final refinement one outlier was omitted (1 2 0).

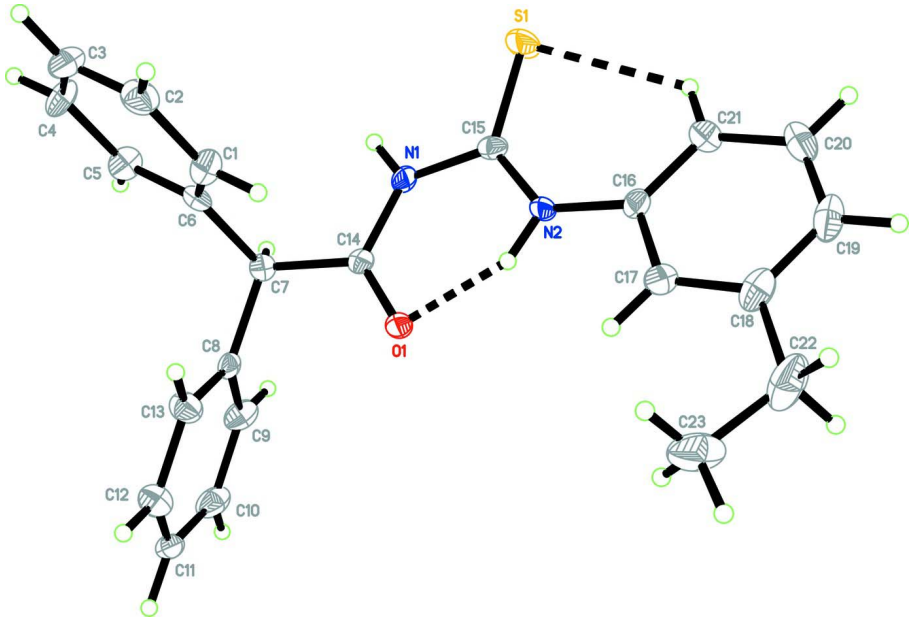

Figure 1

The molecular structure of the title compound shown with 50% probability displacement ellipsoids. Dashed lines represent intramolecular hydrogen bonds.

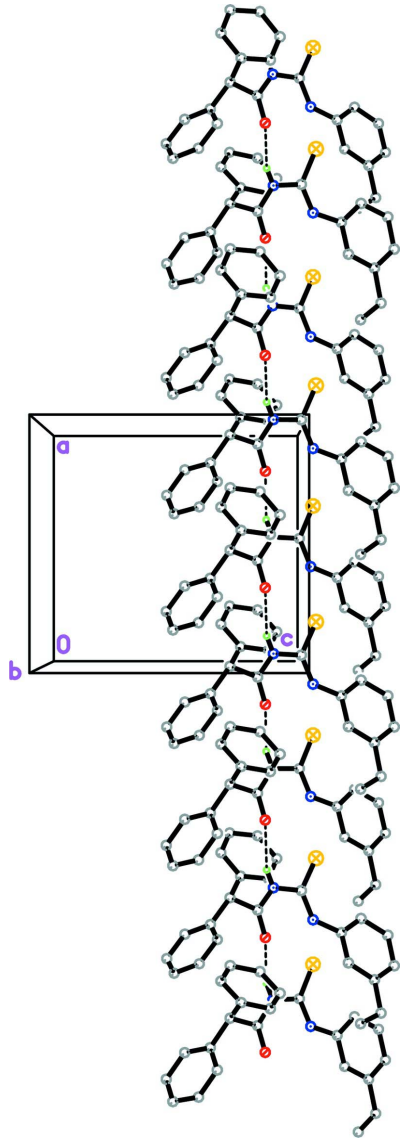

Figure 2

The crystal packing of the title compound. The H atoms not involved in the intermolecular hydrogen bonds (dashed lines) have been omitted for clarity.

N-[(3-Ethylphenyl)carbamothioyl]-2,2-diphenylacetamide

Crystal data

$C_{23}H_{22}N_2OS$
$M_r = 374.49$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 10.0608\ (2)$ Å
$b = 17.9092\ (5)$ Å
$c = 10.8495\ (3)$ Å
$V = 1954.87\ (9)$ Å^3
$Z = 4$
$F(000) = 792$
$D_x = 1.272$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2145 reflections
$\theta = 3.0$–$32.6°$
$\mu = 0.18$ mm^{-1}
$T = 100$ K
Plate, colourless
0.26 × 0.23 × 0.09 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.955, T_{max} = 0.983
11560 measured reflections
4121 independent reflections
2885 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −13→12
k = −23→19
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.098
S = 0.99
4121 reflections
253 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 1761 Friedel pairs
Absolute structure parameter: 0.17 (9)

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.31660 (6)	0.86772 (5)	0.55685 (8)	0.0304 (2)
O1	0.67282 (17)	0.76358 (11)	0.36156 (18)	0.0183 (5)
N1	0.4543 (2)	0.79237 (14)	0.3925 (2)	0.0167 (6)
N2	0.5813 (2)	0.84342 (13)	0.5464 (2)	0.0171 (6)
C1	0.4471 (3)	0.60946 (17)	0.3775 (3)	0.0228 (8)
H1A	0.5140	0.6275	0.4317	0.027*
C2	0.3680 (3)	0.54945 (18)	0.4134 (3)	0.0273 (8)
H2A	0.3806	0.5270	0.4919	0.033*
C3	0.2716 (3)	0.52269 (19)	0.3353 (3)	0.0288 (9)
H3A	0.2173	0.4819	0.3599	0.035*
C4	0.2539 (3)	0.55506 (19)	0.2211 (3)	0.0267 (8)
H4A	0.1879	0.5362	0.1667	0.032*
C5	0.3322 (3)	0.61505 (17)	0.1855 (3)	0.0218 (7)

H5A	0.3193	0.6373	0.1069	0.026*
C6	0.4296 (3)	0.64289 (17)	0.2643 (3)	0.0159 (7)
C7	0.5123 (3)	0.70924 (15)	0.2215 (3)	0.0151 (6)
H7A	0.4535	0.7410	0.1689	0.018*
C8	0.6323 (3)	0.68784 (16)	0.1434 (3)	0.0153 (7)
C9	0.6652 (3)	0.73113 (17)	0.0418 (3)	0.0228 (7)
H9A	0.6124	0.7734	0.0217	0.027*
C10	0.7742 (3)	0.7136 (2)	−0.0309 (3)	0.0269 (8)
H10A	0.7961	0.7440	−0.0997	0.032*
C11	0.8512 (3)	0.65166 (19)	−0.0030 (3)	0.0260 (8)
H11A	0.9252	0.6390	−0.0532	0.031*
C12	0.8195 (3)	0.60861 (19)	0.0980 (3)	0.0289 (8)
H12A	0.8725	0.5664	0.1180	0.035*
C13	0.7102 (3)	0.62655 (18)	0.1710 (3)	0.0229 (7)
H13A	0.6891	0.5964	0.2404	0.028*
C14	0.5563 (3)	0.75715 (16)	0.3310 (3)	0.0133 (6)
C15	0.4590 (3)	0.83515 (16)	0.5009 (3)	0.0161 (7)
C16	0.6292 (3)	0.87797 (16)	0.6550 (3)	0.0174 (7)
C17	0.7605 (3)	0.86083 (17)	0.6841 (3)	0.0228 (8)
H17A	0.8072	0.8263	0.6336	0.027*
C18	0.8250 (3)	0.89224 (18)	0.7834 (3)	0.0262 (8)
C19	0.7545 (3)	0.94264 (19)	0.8556 (3)	0.0290 (8)
H19A	0.7969	0.9658	0.9238	0.035*
C20	0.6235 (3)	0.95954 (19)	0.8292 (3)	0.0279 (8)
H20A	0.5763	0.9934	0.8805	0.034*
C21	0.5598 (3)	0.92747 (17)	0.7284 (3)	0.0215 (7)
H21A	0.4699	0.9395	0.7103	0.026*
C22	0.9695 (3)	0.8747 (2)	0.8103 (4)	0.0425 (11)
H22A	0.9778	0.8621	0.8989	0.051*
H22B	1.0225	0.9204	0.7956	0.051*
C23	1.0305 (3)	0.8111 (2)	0.7353 (3)	0.0440 (11)
H23A	1.1230	0.8036	0.7608	0.066*
H23B	1.0277	0.8239	0.6475	0.066*
H23C	0.9799	0.7652	0.7495	0.066*
H1N1	0.379 (3)	0.7853 (15)	0.366 (3)	0.019 (9)*
H1N2	0.640 (3)	0.8181 (17)	0.500 (3)	0.025 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0143 (3)	0.0422 (5)	0.0348 (5)	0.0050 (4)	0.0033 (4)	−0.0157 (5)
O1	0.0112 (9)	0.0225 (12)	0.0212 (11)	0.0009 (9)	−0.0011 (10)	−0.0068 (10)
N1	0.0095 (12)	0.0191 (15)	0.0214 (15)	−0.0001 (11)	−0.0041 (12)	−0.0051 (12)
N2	0.0100 (11)	0.0222 (14)	0.0191 (13)	0.0018 (10)	0.0008 (13)	−0.0076 (14)
C1	0.0232 (17)	0.0190 (19)	0.0263 (19)	−0.0023 (14)	−0.0034 (15)	0.0008 (16)
C2	0.035 (2)	0.025 (2)	0.0213 (17)	0.0008 (16)	0.0088 (16)	0.0028 (17)
C3	0.0222 (16)	0.026 (2)	0.039 (2)	−0.0070 (14)	0.0067 (18)	0.0000 (18)
C4	0.0216 (16)	0.027 (2)	0.0316 (19)	−0.0109 (15)	−0.0075 (16)	−0.0021 (18)

C5	0.0221 (16)	0.025 (2)	0.0177 (16)	−0.0007 (14)	−0.0055 (14)	0.0040 (15)
C6	0.0173 (15)	0.0175 (18)	0.0130 (15)	0.0045 (13)	0.0037 (13)	−0.0005 (14)
C7	0.0157 (14)	0.0151 (16)	0.0144 (15)	0.0010 (12)	−0.0018 (13)	0.0006 (14)
C8	0.0161 (14)	0.0185 (17)	0.0114 (15)	−0.0049 (13)	−0.0016 (13)	−0.0035 (14)
C9	0.0164 (15)	0.0286 (18)	0.0233 (17)	−0.0023 (13)	−0.0078 (15)	0.0042 (17)
C10	0.0249 (17)	0.037 (2)	0.0183 (18)	−0.0127 (15)	0.0014 (15)	0.0005 (17)
C11	0.0171 (15)	0.035 (2)	0.0259 (19)	−0.0096 (15)	0.0067 (15)	−0.0141 (18)
C12	0.0235 (17)	0.0252 (19)	0.038 (2)	0.0031 (15)	0.0038 (17)	−0.0054 (17)
C13	0.0240 (16)	0.0197 (18)	0.0251 (18)	0.0020 (13)	0.0051 (14)	0.0009 (16)
C14	0.0157 (13)	0.0101 (16)	0.0140 (14)	−0.0014 (12)	0.0021 (13)	0.0044 (13)
C15	0.0142 (14)	0.0149 (17)	0.0192 (16)	−0.0001 (12)	0.0033 (13)	0.0034 (15)
C16	0.0176 (14)	0.0153 (17)	0.0192 (17)	−0.0038 (13)	0.0002 (14)	−0.0003 (15)
C17	0.0189 (15)	0.0226 (19)	0.0269 (18)	−0.0020 (14)	0.0027 (15)	−0.0025 (16)
C18	0.0278 (16)	0.0238 (19)	0.0269 (18)	−0.0064 (15)	−0.0091 (16)	0.0055 (17)
C19	0.044 (2)	0.025 (2)	0.0185 (16)	−0.0138 (17)	−0.0059 (17)	0.0016 (17)
C20	0.0384 (18)	0.025 (2)	0.0202 (17)	0.0013 (16)	0.0034 (17)	−0.0042 (16)
C21	0.0225 (15)	0.0230 (19)	0.0190 (16)	0.0021 (14)	0.0013 (15)	−0.0007 (16)
C22	0.036 (2)	0.038 (2)	0.053 (3)	−0.0038 (18)	−0.024 (2)	−0.004 (2)
C23	0.0202 (18)	0.086 (3)	0.025 (2)	0.004 (2)	−0.0051 (16)	0.003 (2)

Geometric parameters (Å, º)

S1—C15	1.662 (3)	C9—H9A	0.9500
O1—C14	1.224 (3)	C10—C11	1.386 (5)
N1—C14	1.377 (3)	C10—H10A	0.9500
N1—C15	1.404 (4)	C11—C12	1.378 (4)
N1—H1N1	0.82 (3)	C11—H11A	0.9500
N2—C15	1.334 (3)	C12—C13	1.393 (4)
N2—C16	1.416 (4)	C12—H12A	0.9500
N2—H1N2	0.90 (3)	C13—H13A	0.9500
C1—C6	1.378 (4)	C16—C21	1.381 (4)
C1—C2	1.393 (4)	C16—C17	1.391 (4)
C1—H1A	0.9500	C17—C18	1.379 (4)
C2—C3	1.374 (4)	C17—H17A	0.9500
C2—H2A	0.9500	C18—C19	1.389 (5)
C3—C4	1.380 (5)	C18—C22	1.516 (4)
C3—H3A	0.9500	C19—C20	1.383 (4)
C4—C5	1.387 (4)	C19—H19A	0.9500
C4—H4A	0.9500	C20—C21	1.392 (4)
C5—C6	1.392 (4)	C20—H20A	0.9500
C5—H5A	0.9500	C21—H21A	0.9500
C6—C7	1.523 (4)	C22—C23	1.528 (5)
C7—C8	1.524 (4)	C22—H22A	0.9900
C7—C14	1.531 (4)	C22—H22B	0.9900
C7—H7A	1.0000	C23—H23A	0.9800
C8—C13	1.382 (4)	C23—H23B	0.9800
C8—C9	1.388 (4)	C23—H23C	0.9800
C9—C10	1.387 (4)		

C14—N1—C15	129.1 (2)	C11—C12—C13	120.4 (3)
C14—N1—H1N1	117 (2)	C11—C12—H12A	119.8
C15—N1—H1N1	114 (2)	C13—C12—H12A	119.8
C15—N2—C16	132.1 (3)	C8—C13—C12	120.5 (3)
C15—N2—H1N2	109.9 (18)	C8—C13—H13A	119.7
C16—N2—H1N2	117.7 (18)	C12—C13—H13A	119.7
C6—C1—C2	120.7 (3)	O1—C14—N1	122.6 (3)
C6—C1—H1A	119.6	O1—C14—C7	122.7 (2)
C2—C1—H1A	119.6	N1—C14—C7	114.7 (2)
C3—C2—C1	120.0 (3)	N2—C15—N1	113.7 (2)
C3—C2—H2A	120.0	N2—C15—S1	128.4 (2)
C1—C2—H2A	120.0	N1—C15—S1	117.9 (2)
C2—C3—C4	119.9 (3)	C21—C16—C17	119.4 (3)
C2—C3—H3A	120.0	C21—C16—N2	126.0 (3)
C4—C3—H3A	120.0	C17—C16—N2	114.5 (3)
C3—C4—C5	120.1 (3)	C18—C17—C16	122.3 (3)
C3—C4—H4A	119.9	C18—C17—H17A	118.9
C5—C4—H4A	119.9	C16—C17—H17A	118.9
C4—C5—C6	120.4 (3)	C17—C18—C19	117.7 (3)
C4—C5—H5A	119.8	C17—C18—C22	121.2 (3)
C6—C5—H5A	119.8	C19—C18—C22	121.0 (3)
C1—C6—C5	118.8 (3)	C20—C19—C18	120.8 (3)
C1—C6—C7	122.7 (3)	C20—C19—H19A	119.6
C5—C6—C7	118.5 (3)	C18—C19—H19A	119.6
C6—C7—C8	114.0 (2)	C19—C20—C21	120.7 (3)
C6—C7—C14	111.0 (2)	C19—C20—H20A	119.6
C8—C7—C14	110.1 (2)	C21—C20—H20A	119.6
C6—C7—H7A	107.1	C16—C21—C20	119.0 (3)
C8—C7—H7A	107.1	C16—C21—H21A	120.5
C14—C7—H7A	107.1	C20—C21—H21A	120.5
C13—C8—C9	118.7 (3)	C18—C22—C23	115.9 (3)
C13—C8—C7	121.9 (3)	C18—C22—H22A	108.3
C9—C8—C7	119.4 (3)	C23—C22—H22A	108.3
C10—C9—C8	120.9 (3)	C18—C22—H22B	108.3
C10—C9—H9A	119.5	C23—C22—H22B	108.3
C8—C9—H9A	119.5	H22A—C22—H22B	107.4
C11—C10—C9	120.0 (3)	C22—C23—H23A	109.5
C11—C10—H10A	120.0	C22—C23—H23B	109.5
C9—C10—H10A	120.0	H23A—C23—H23B	109.5
C12—C11—C10	119.5 (3)	C22—C23—H23C	109.5
C12—C11—H11A	120.3	H23A—C23—H23C	109.5
C10—C11—H11A	120.3	H23B—C23—H23C	109.5

C6—C1—C2—C3	0.4 (5)	C15—N1—C14—O1	−5.2 (5)
C1—C2—C3—C4	0.3 (5)	C15—N1—C14—C7	174.6 (3)
C2—C3—C4—C5	−0.7 (5)	C6—C7—C14—O1	114.1 (3)
C3—C4—C5—C6	0.3 (5)	C8—C7—C14—O1	−13.1 (4)

C2—C1—C6—C5	−0.8 (4)	C6—C7—C14—N1	−65.8 (3)
C2—C1—C6—C7	179.2 (3)	C8—C7—C14—N1	167.0 (2)
C4—C5—C6—C1	0.4 (4)	C16—N2—C15—N1	−176.0 (3)
C4—C5—C6—C7	−179.5 (3)	C16—N2—C15—S1	3.2 (5)
C1—C6—C7—C8	94.9 (3)	C14—N1—C15—N2	2.0 (4)
C5—C6—C7—C8	−85.2 (3)	C14—N1—C15—S1	−177.3 (2)
C1—C6—C7—C14	−30.1 (4)	C15—N2—C16—C21	−16.1 (5)
C5—C6—C7—C14	149.8 (3)	C15—N2—C16—C17	166.4 (3)
C6—C7—C8—C13	−40.4 (4)	C21—C16—C17—C18	−0.7 (4)
C14—C7—C8—C13	85.1 (3)	N2—C16—C17—C18	177.0 (3)
C6—C7—C8—C9	139.9 (3)	C16—C17—C18—C19	−0.1 (5)
C14—C7—C8—C9	−94.6 (3)	C16—C17—C18—C22	−177.8 (3)
C13—C8—C9—C10	−0.1 (4)	C17—C18—C19—C20	1.0 (5)
C7—C8—C9—C10	179.6 (3)	C22—C18—C19—C20	178.7 (3)
C8—C9—C10—C11	0.6 (4)	C18—C19—C20—C21	−1.2 (5)
C9—C10—C11—C12	−0.9 (4)	C17—C16—C21—C20	0.5 (4)
C10—C11—C12—C13	0.7 (4)	N2—C16—C21—C20	−176.8 (3)
C9—C8—C13—C12	−0.1 (4)	C19—C20—C21—C16	0.4 (4)
C7—C8—C13—C12	−179.8 (3)	C17—C18—C22—C23	−10.1 (5)
C11—C12—C13—C8	−0.2 (4)	C19—C18—C22—C23	172.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*N*2···O1	0.90 (3)	1.82 (3)	2.630 (3)	148 (3)
C21—H21*A*···S1	0.95	2.61	3.255 (3)	126
N1—H1*N*1···O1^{i}	0.82 (3)	2.25 (3)	3.023 (3)	157 (3)
C7—H7*A*···*Cg*^{ii}	1.00	2.87	3.844 (3)	166

Symmetry codes: (i) *x*−1/2, −*y*+3/2, *z*; (ii) −*x*−1/2, *y*+3/2, *z*+1/2.